LA-UR-19-22247
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Title: Overview of DOE-NE NEAMS Program

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Intended for: Report

Issued: 2019-03-13

U.S. DEPARTMENT OF ENERGY | Office of NUCLEAR ENERGY

Clean. Reliable. Nuclear.

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Overview of DOE-NE NEAMS Program

NEAMS

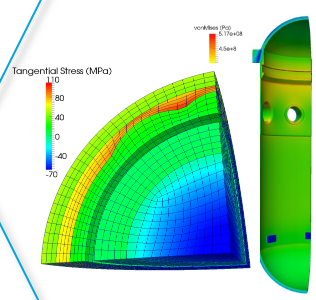
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

NEAMS Overview

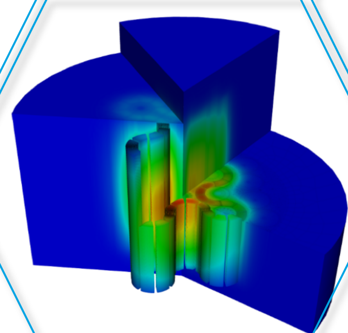
The NEAMS (Nuclear Energy Advanced Modeling and Simulation) program is a multi-national lab team effort aiming to develop and deploy predictive computer methods for the analysis and design of advanced nuclear reactors.

US Department of Energy has made significant investments in advanced mod-sim during last decade between CASL and NEAMS. Next year, aim is for all NE mod sim to be centralized in a single program.

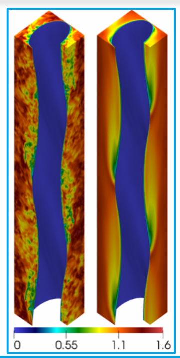
NEAMS core competencies:



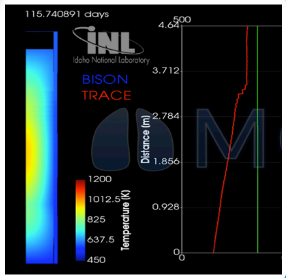
Multiscale fuel performance and structural materials degradation modeling:
BISON, GRIZZLY



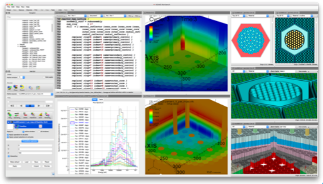
Reactor Physics:
PROTEUS, MAMMOTH



Multiscale thermal fluids:
SAM, PRONGHORN, Sockeye, Nek5000



Multiphysics:
MOOSE

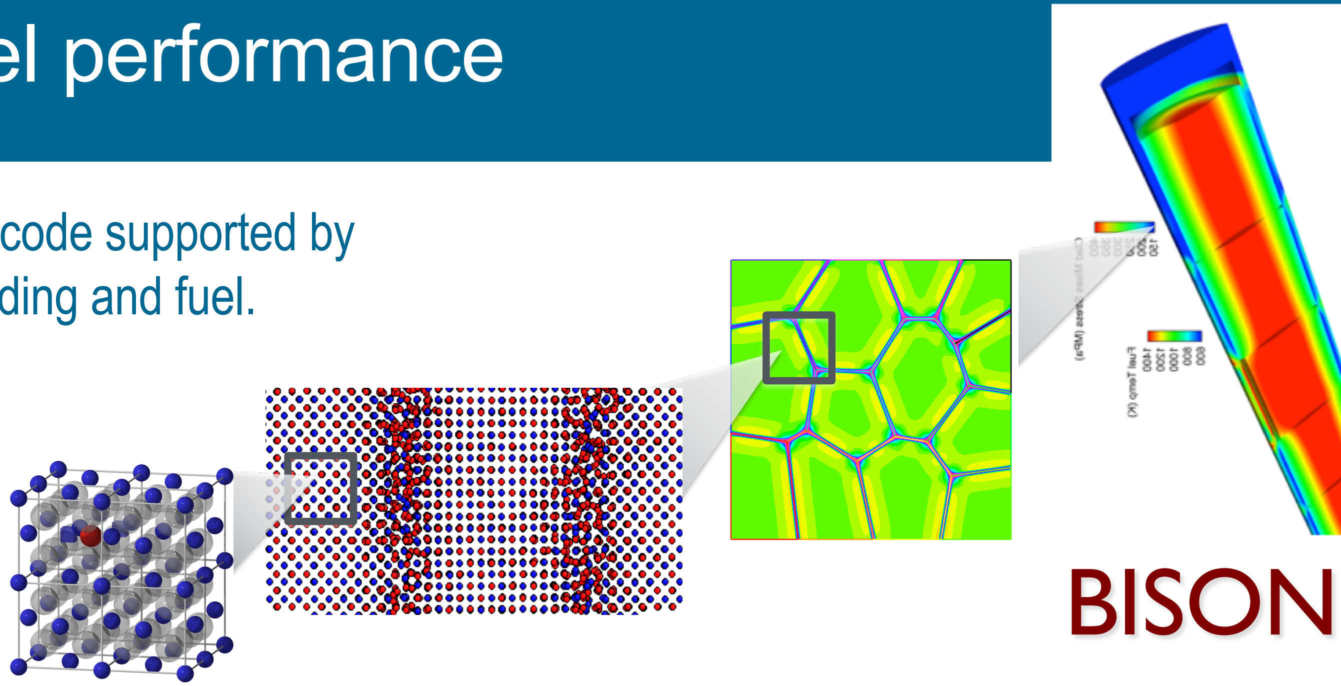


Workflow Management:
Workbench

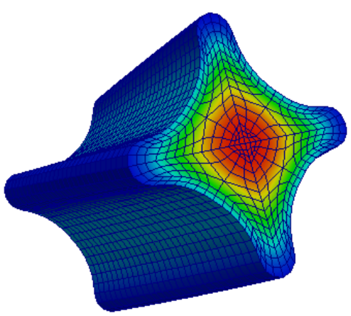
Multiscale fuel performance

BISON fuel performance code supported by multiscale studies of cladding and fuel.

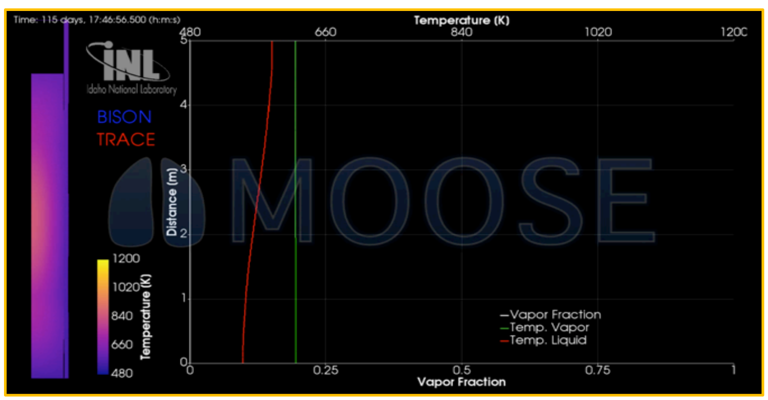
Insight gained at lower length scales incorporated in to BISON via constitutive equations, models, parameters, etc.



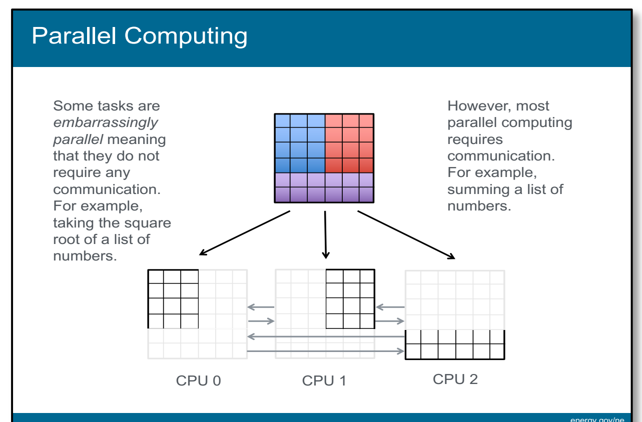
Other key advantages of BISON



3D Fuel Performance



Multiphysics Coupling



Parallel Computing

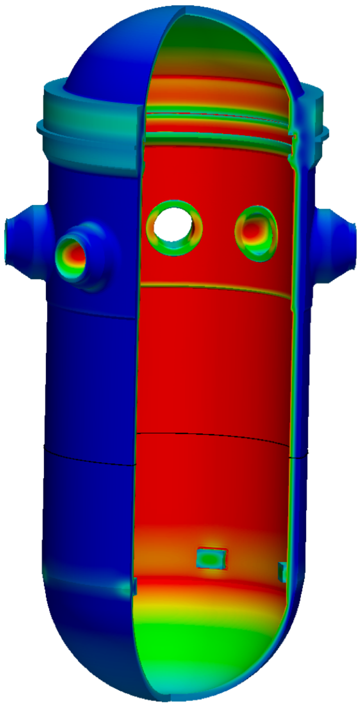
FY19 Plans – Fuel Performance

Transition from UO_2 and ATF to Advanced Reactor Fuel

- **Metallic fuel capability**
  - Model development: swelling and FCCI
  - Validation plan including new validation cases
  - Develop and distribute ANL out-of-pile validation database
  - Support for MW-scale demonstration problem and commercial designers
- **TRISO particle fuel capability**
  - Training and model development support for industry collaborators
  - Particle failure probabilities (failure models and statistical treatment)
  - Validation plan including new validation cases
  - Develop diffusion parameters for UCO fission gas release models
- **General fuel performance**
  - Improvements to frictional contact capability and code robustness
  - Adapt XFEM to simulate moving material interface
  - Improve code documentation and testing
  - User training and support

Grizzly: Introduction and FY19 Plans

- What is **Grizzly**?
  - MOOSE-based simulation tool for aging in nuclear power plant systems, components, and structures
  - Used to model both aging processes and the ability of age-degraded components to safely function
  - Selected by **Kairos Power** for vessel design/licensing
  - Development team recently provided full-day overview and training at NRC: clear interest for advanced reactors
- Development/application plans for advanced reactors:
  - Engineering-scale material models (creep/plasticity) appropriate for high temperatures
  - Engineering-scale models that incorporate the behavior of a visco-plastic self consistent material model represented through a reduced order model
  - Further development of the extended finite element method (XFEM) capability to permit crack propagation in 3D models of structural components

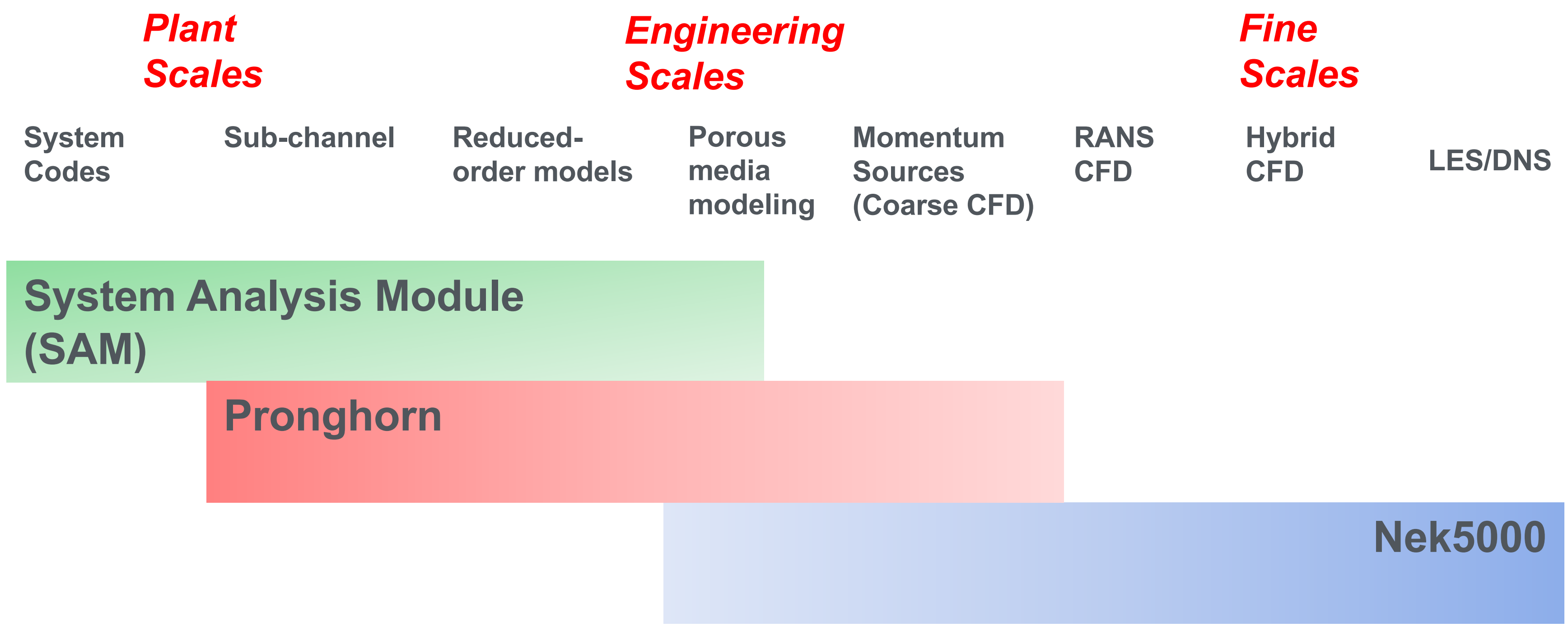


B. Spencer, et al. "Modular system for probabilistic fracture mechanics analysis of embrittled reactor pressure vessels in the Grizzly code," *Nuc Eng Des*, **341**:25 (2019)

Overview of Thermal-hydraulic capabilities

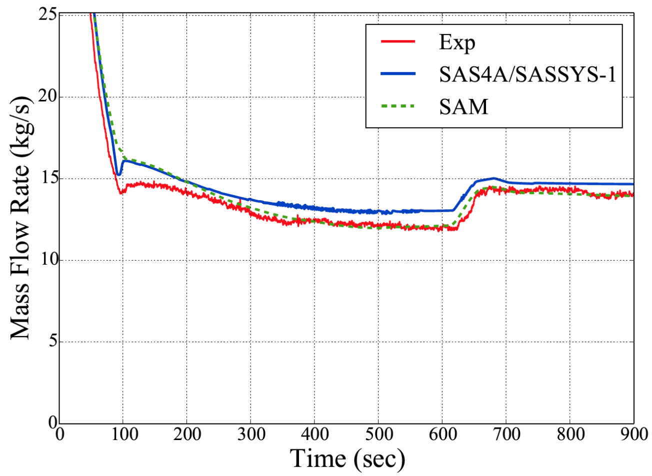
Background

- DOE is developing modern multiscale thermal-hydraulic (T/H) tools applicable to a variety of advanced reactor concepts
- While validation focus has been primarily on Sodium Fast Reactors and Gas Reactors to date, the validation basis is being extended to other designs.
- Due to massive scale separation in nuclear systems a multiscale approach is desirable.

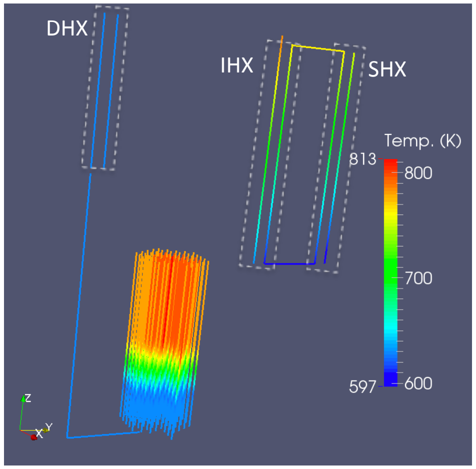


SAM: Overview

- A modern plant-level system analysis tool for advanced reactors in liquid form (SFR, LFR, MSR/FHR) safety analysis. Some application to Gas reactors.
- Advances in software environments and design (MOOSE), numerical methods, and physical models.
- Focused on system T/H.
- **Enhancements in large volume modeling**: 0D, 1D stratification models and full 3D modeling (porous media).
- **Enhancements in core modeling**: Single-channel, Multiple-Channel and Intermediate fidelity (targeted toward SFR) core modeling.
- **Enhancements related to MSRs**: delayed neutron precursors transport, freeze and thaw models.
- **Flexible multi-scale multi-physics.**



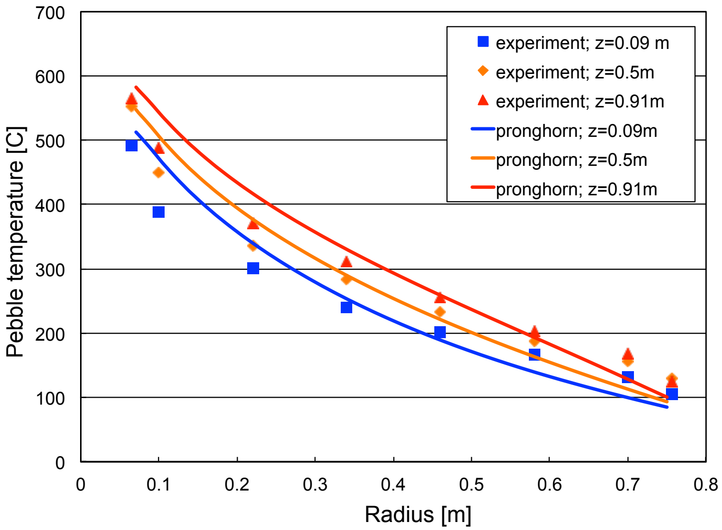
Mass flow rate in EBR-II SHRT-45R Benchmark



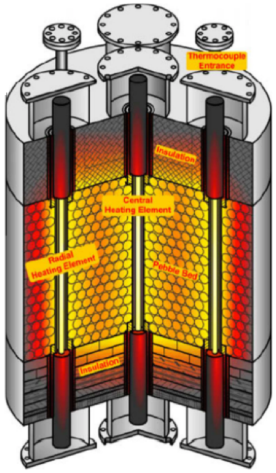
Representation of a PLOF in ABTR

Pronghorn: Overview

- A modern engineering-level system analysis tool for advanced reactors.
- Advances in software environments and design (MOOSE), numerical methods, and physical models.
- Targeting primarily pebble bed reactors (FHR/HTGR) but extendable to other designs.
- Anisotropic porous media modeling as we well as more advanced formulations.
- **Enhanced formulation**: It can combine porous media regions with open regions. Flexible multi-scale multi-physics.
  - It can be described as homogenized conjugate heat transfer (CHT), where each finite element may contain a mixture of coolant, fuel, moderator, or other core internals.
  - Correlations for anisotropic resistance from Nek5000 can be implemented in a straightforward manner.
- **Coupling to SAM for RCCS modeling.**

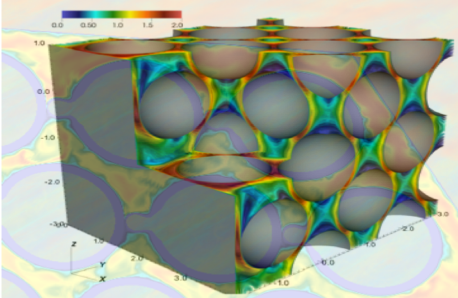


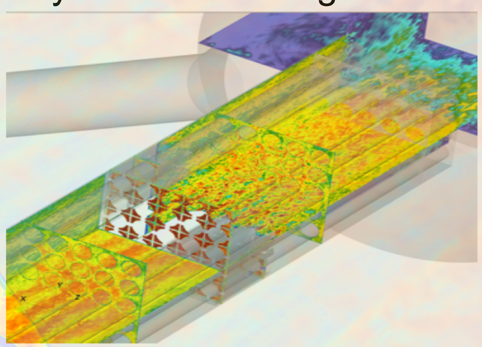
Comparison between Pronghorn and SANA dataset. Pebble temperature at various axial locations.

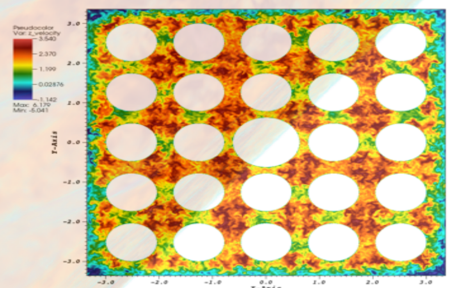


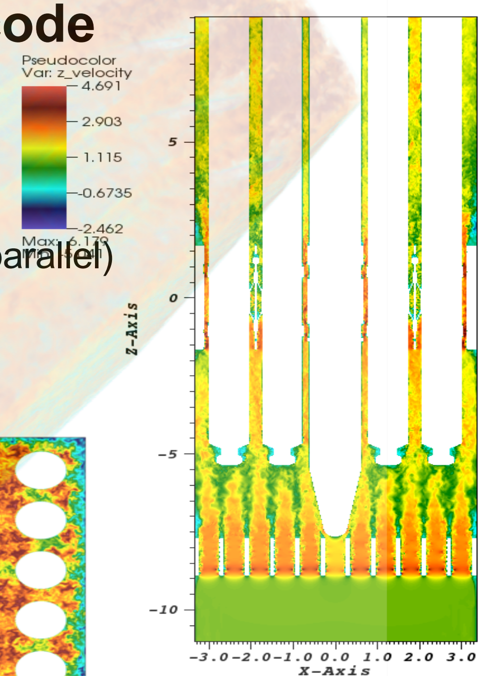
B. Stocker and H. Nieben. Data Sets of the SANA Experiment 1994–1996. Technical report, Forschungszentrum Julich, 1996.

- **Spectral element, computational fluid dynamics code**
  - Open Source
  - Accepts meshes in a variety of formats
    - *2D or 3D*
  - Runs on platforms ranging from laptops to supercomputer (massively parallel)
  - R&D100 Award (2016)
  - Couples to other analysis codes through MOOSE

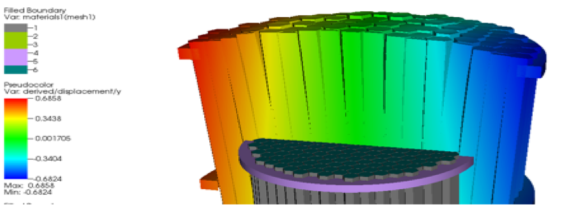




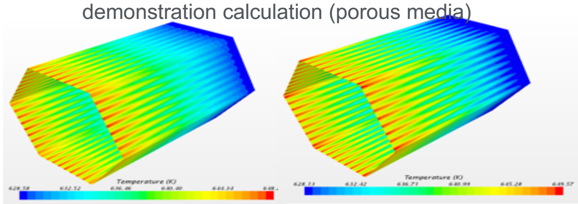




Nek5000: What can it do?



Full core SHARP's Nek5000-Proteus-Diablo demonstration calculation (porous media)

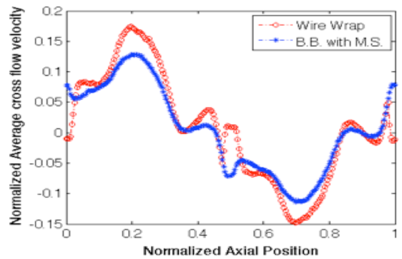


Porous media 3-region model

CFD

Porous Media ~1x

Resolves only the largest scale with reduced geometric complexity. Low computational cost. Can reach full core on a cluster. Small cases can run on a laptop.

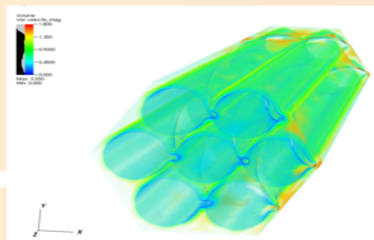


Momentum sources/ Coarse CFD ~20x

Resolves only the largest scale with reduced geometric complexity. Medium to low computational cost. Benefits from the scalability of Nek5000. Maximum size typically covers a portion to a full fuel assembly on a cluster. Can reach full core.

(u)RANS ~200x

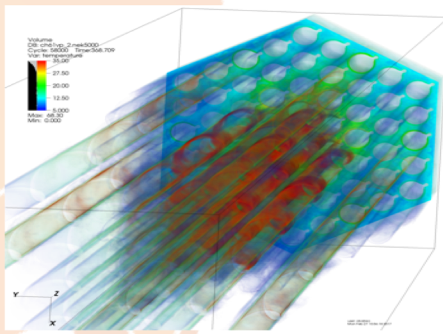
Resolves only the largest scale. Medium computational cost. Benefits from the scalability of Nek5000. Maximum size typically covers a portion to a full .



7-pin wire-wrapped calculation (single pitch). RANS

LES/DNS ~>10,000x

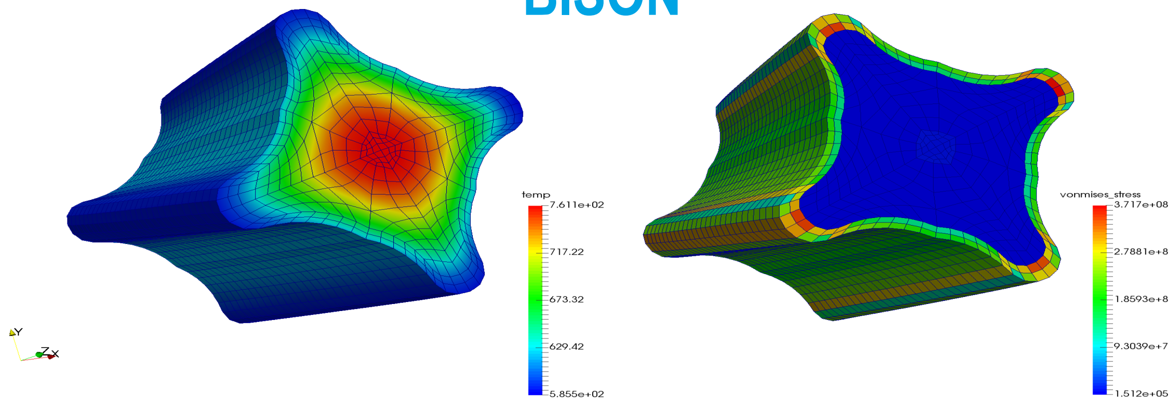
Resolves most to all of relevant scales. High computational cost. Benefits from the scalability of Nek5000. Maximum size typically covers a portion to a full fuel assembly on a supercomputer.



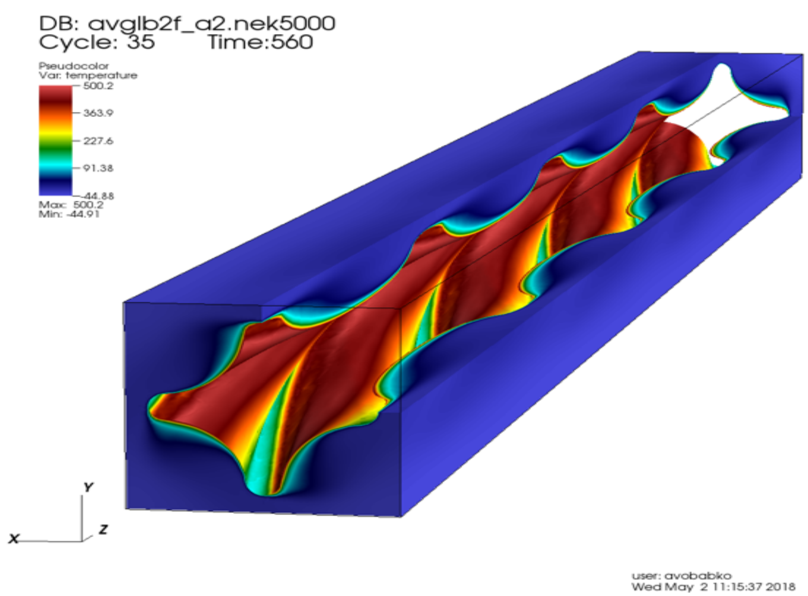
61-pin wire-wrapped LES of AREVA/Terrapower 7-pitch bunddle (**1M MPI ranks**)

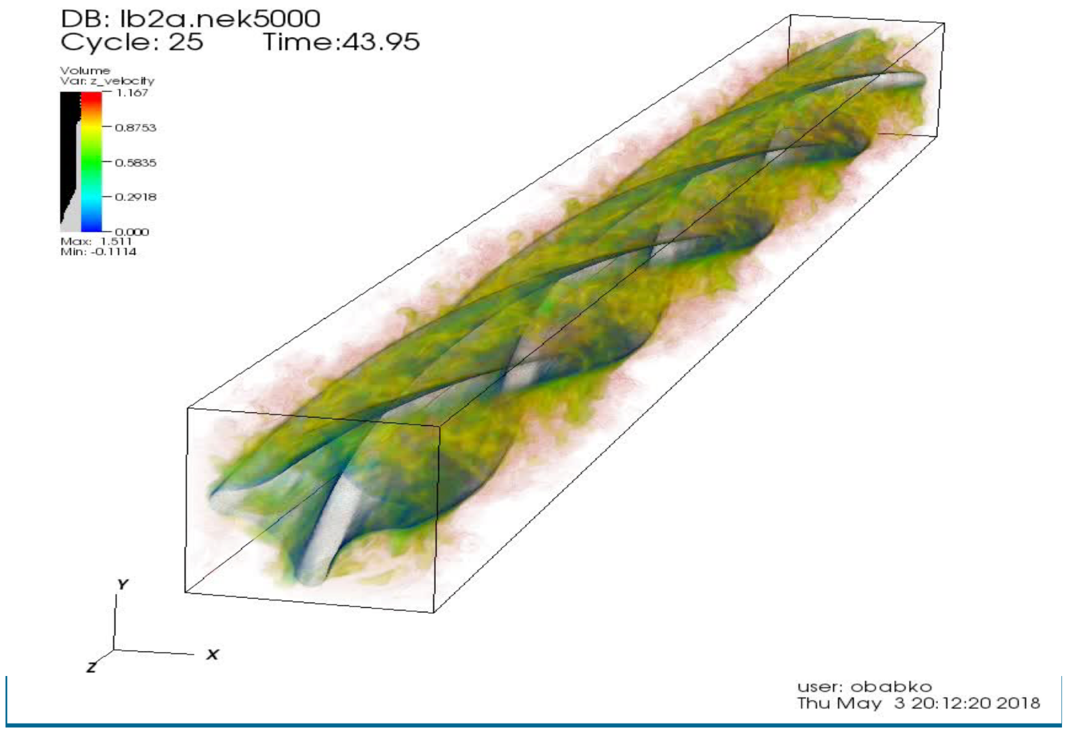
Ability to Model Advanced Fuel/ATF:
Lightbridge w/ BISON-Nek5000 (uncoupled)

BISON



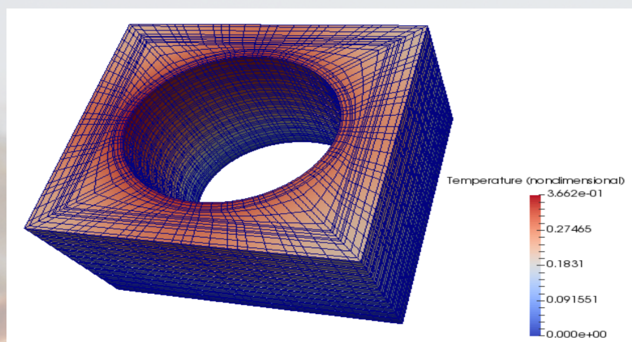
Nek5000

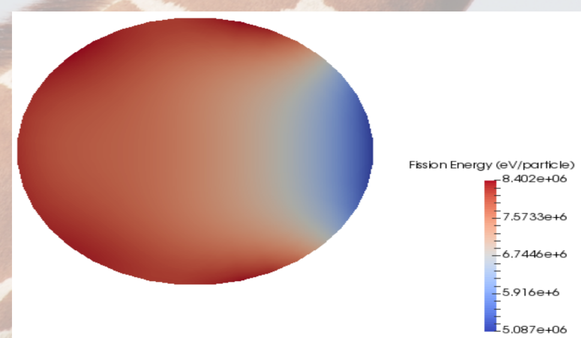




Coupling Nek5000 to MOOSE:
Giraffe

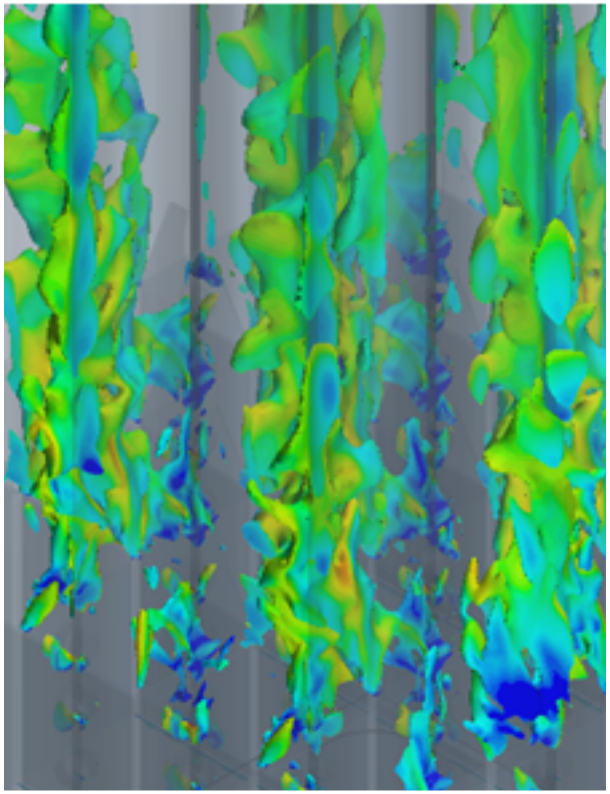
- A MOOSE-based coupling interface for Nek5000
  - Intended for multiphysics feedback in reactor simulations
    - Temperature
    - Density
    - Flux at boundaries
  - Currently demonstrated coupling with:
    - Giraffe + Okapi + Buffalo (**Bison's proxy**) coupling (April Novak, UC Berkeley)
    - Systems-level safety (SAM) analysis (Rui Hu, ANL)





Overview of center of excellence for T/F applications in nuclear energy

- **Mission**: Provides leadership, best practices, research, support and training for thermal-fluids research in nuclear energy
- **Launched in April 2018 with a kickoff workshop**
- **How?** Researching advanced algorithms and developing modern software tools for solving challenging fluid flow problems
  - Typically, fluid dynamic spatial and temporal scales for nuclear power application can span ten orders of magnitude.
  - **External forces and sources** of mass and energy (FSI/corrosion/MHD) in some way influence all flow domains.
  - These new solution strategies and algorithms will be implemented eventually into a NQA-1 level software and validation campaigns will be undertaken
- **Why?** The center addresses a pressing need in advanced reactor development and commercialization.
  - Advanced reactor fluid problems are currently high priority and lend themselves to advanced modeling and simulation due to the lack of empirical data
  - T/H issues with Advanced Fuels.

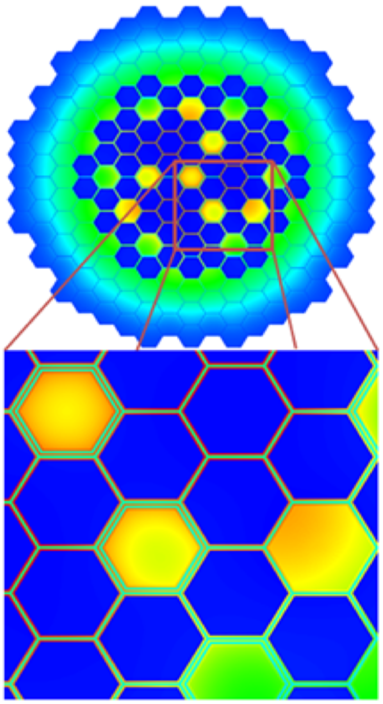


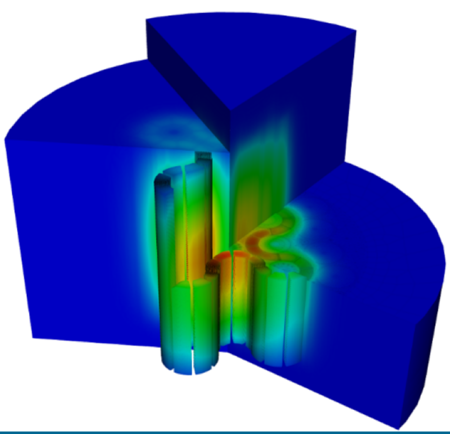
Isosurfaces of the velocity in a 5x5 grid spacer

Core Physics Overview

- DOE's Nuclear Energy Advanced Modeling and Simulation program supports development of high-fidelity capable neutron transport code suite for advanced reactors
  - Deterministic tools to complement Monte Carlo techniques by compensating for their limitations
    - Transient analyses with deforming mesh
    - Fine-grid flux distributions for rigorous treatment of multi-physics phenomena
    - Shielding and dose rate calculations in regions with low flux
  - High-fidelity capability extends application regime to complex geometries and sharply heterogeneous material compositions
- Desired impact
  - Improved operational and safety margins through higher-order modeling
  - "Close to first principles" solutions for benchmarking lower-fidelity/order modeling approaches
  - Multi-physics interface with matching levels of fidelity
  - Enhance the impact of experiments to support reactor design/licensing

PROTEUS Neutronics Suite





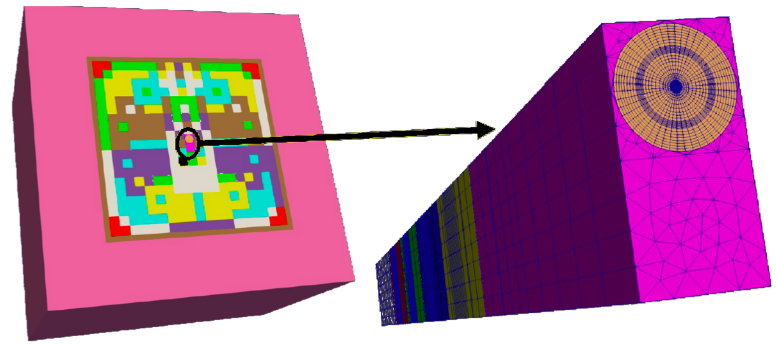
- Complete package with unstructured finite element meshing tools, range of multi-group cross-section generation options (for both thermal and fast spectrum), neutron/radiation transport solvers, depletion and sensitivity analyses, and post-processing capabilities
  - Multi-physics interface for thermal and core deformation feedback
- **MC^2-3 and Cross Section API**: For high-quality multi-group cross section generation with local heterogeneity effects
  - https://www.anl.gov/technology/project/mc2-3-multigroup-cross-sections-fast-reactors
- **PROTEUS**: Two high-fidelity, highly-scalable neutron transport solver options (SN and MOC) and a nodal transport solver option (NODAL)
  - https://www.ne.anl.gov/codes/proteus/
- **PERSENT**: Perturbation and sensitivity analyses based on the variational nodal transport method (to determine reactivity feedback coefficients)

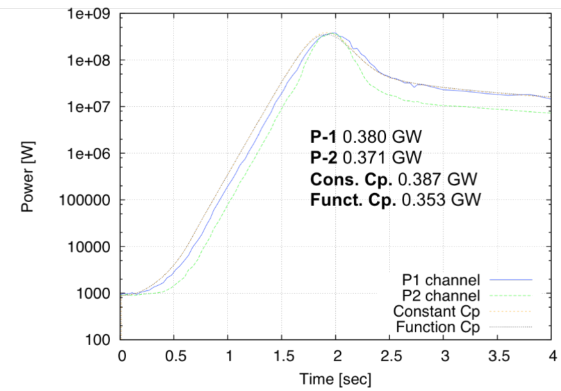
RattleSnake

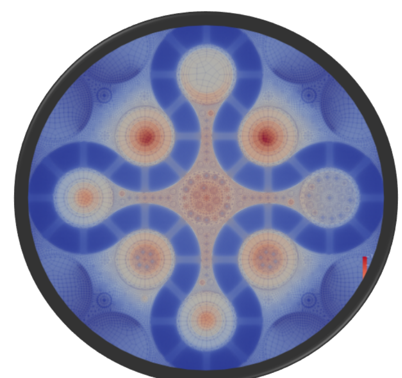
A multi-scheme radiation transport application

Deterministic radiation transport solver for linearized time-dependent Boltzmann radiation transport equation

- Originally developed to support TREAT reactor restart and experiment modeling, based on a finite element solver for SN and PN approximations
- Designed for tightly coupled nonlinear multiphysics simulations to capture the impact of temperature and material density changes on time-dependent flux distribution, reaction rates, and power profile
- Multi-scheme capability for a fine-scale resolution in places where interesting multiphysics phenomena take place
  - Uses a lower order and/or homogenized solution for less interesting areas
- Lattice, pebble bed and hexagonal fuels, complex configurations such as Advanced Test Reactor (ATR) and the Transient Reactor Test Facility (TREAT)
- https://rattlesnake.inl.gov/SitePages/Home.aspx







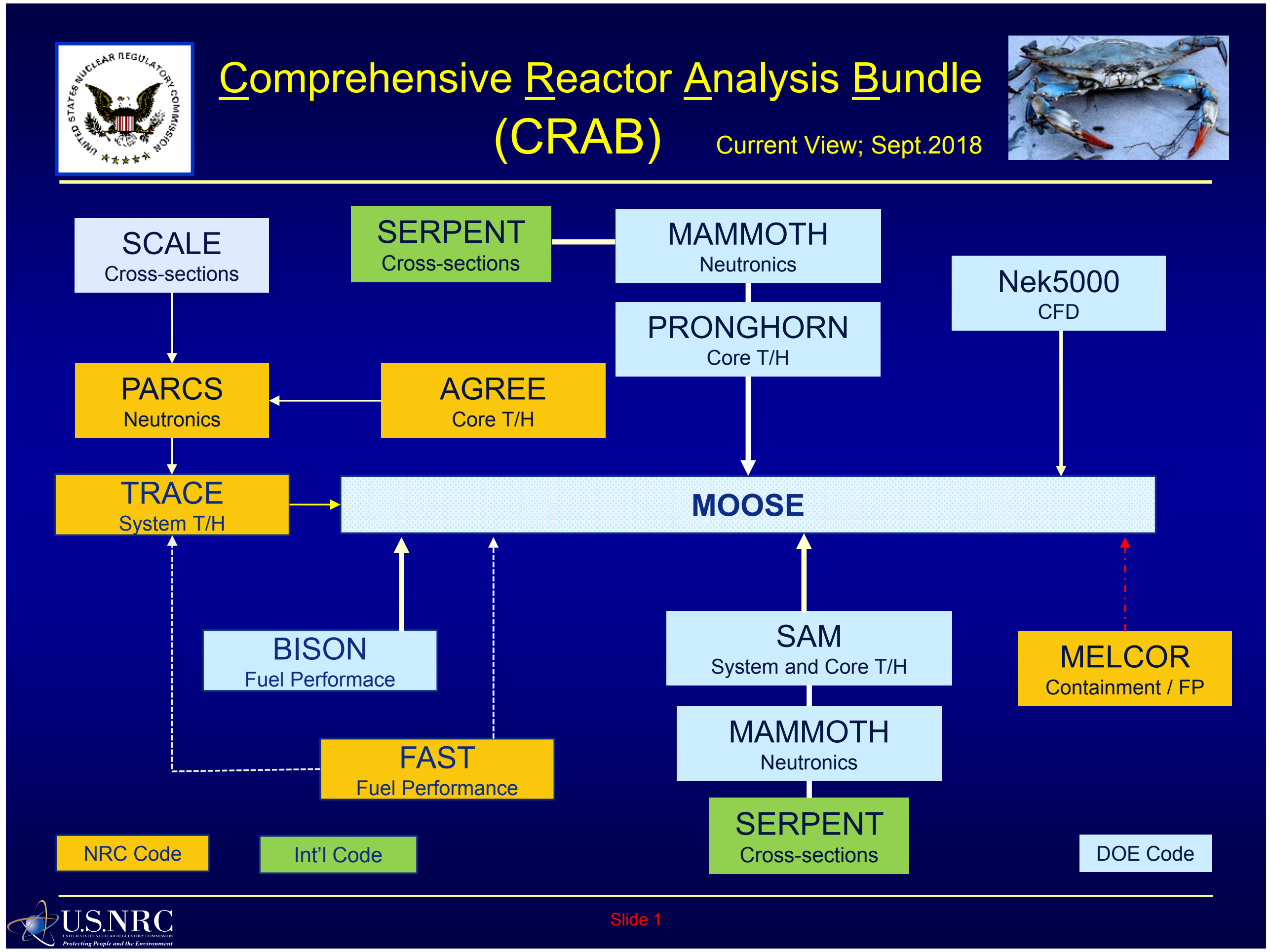
All DOE Codes Invoked in CRAB Vision are Actively Supported by NEAMS

NRC may be open to using codes that did not originate with NRC.

May be possible to maintain independence if NRC and applicant use the same code.

Need for experimental testing may be reduced by high fidelity codes.

CRAB is for licensing confirmatory analysis. Still need for e.g. structural materials.



slide courtesy of Steve Bajorek (RES) – and slightly updated from NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy – Strategy 2 Near- Term Implementation Action Plan Progress Report for Fiscal Year 2017 (ML17319A550)

Software Quality and Validation

Software quality and validation: DOE code development efforts place high level of importance on software quality assurance and validation.

- All codes adhere to strict SQA principles.
- DOE performing sufficient validation for there to be confidence in code use. Additional validation required by users for specific applications.

Validation tests continuously added, and plans are consistent with cases identified by NRC as important.

Nuclear Engineering and Design 301 (2016) 232–244

Contents lists available at ScienceDirect

Nuclear Engineering and Design

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Validating the BISON fuel performance code to integral LWR experiments

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[a] Fuel Modeling and Simulation, Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3840, United States
[b] ANATECH Corporation, 5435 Oberlin Dr., San Diego, CA 92121, United States

HIGHLIGHTS

- The BISON multidimensional fuel performance code is being validated to integral LWR experiments.
- Code and solution verification are necessary prerequisites to validation.
- Fuel centerline temperature comparisons through all phases of fuel life are very reasonable.
- Accuracy in predicting fission gas release is consistent with state-of-the-art modeling and the involved uncertainties.

Goal of NEAMS program is NOT to replace experimental data. Rather, use insights derived from advanced mod-sim to perform more meaningful and potentially fewer experiments, gain deeper understanding of governing physics and ultimately accelerate the overall implementation process.

Example: SAM Validation Status and Plan for SFRs
(C = complete, O = ongoing, P = planned)

TEST MATRIX FOR SAM VALIDATION - LMR Applications												
	TAMU-Wire Warpped Fuel Assembly	KIT-KALLA	UW-Sodium Test	UTK-Square Cavity	CEA-SUPERCAVNA	ENEA-NACIE	KTH-TALL/TALL3D	JAEA-PLANTDL	EBR-II	FFTF	Phenix	MONJU
BASIC PHENOMENOLOGICAL MODELS												
Wire-wrap bundle wall drag friction	P	P				P		P	C	O	P	P
Wire-wrap bundle intra-assembly flow	P	P				P		P	P			
Wire-wrap bundle heat transfer		P				P		P	C	O	P	P
Inter-assembly heat transfer		P						P	P	P	P	P
Low Prandtl number fluid convective heat transfer		P	P		P	P	P	P	C	O	P	P
Fluid conduction		P	P		P	P	P	P	C	O	P	P
Parallel channel flow		P						P	C	O	P	P
Wall heat transfer for 0-D components							P		C	O	P	P
Mixed convection		P			P	P		P			P	P
Buyoancy driven flow			P	C	P	P	P	P	C	O	P	P
Mechanistic pump modeling						P		P	P	P	P	P
Pool dynamics			P	C	P	P	P	P	C	O	P	P
Plenum coupling with liquid level tracking									C	O	P	P
Inter-volume mixing			P		P		P	P	C	O	P	P
Reactor kinetics									P	P	P	P
Reactivity feedback									P	P	P	P
Decay heat generation									P	P	P	P
TYPES OF CALCULATIONS												
Single-phase flow trainsient			P		P	P	P	P	C	O	P	P
Transient heatup/cooldown			P		P	P	P	P	C	O	P	P
Pump coast-down						P	P	P	C	O	P	P
Thermal stratification			P		P		P	P	C	O	P	P
Transition to natural circulation						P	P	P	C	O	P	P
Subassembly flow redistribution						P			P			
Core flow redistribution									C	O	P	P
Coupled system and CFD code simulation							P	P	P			P
Coupled with spatial kinetics code simulation									P	P		
Numerical convergence							P	P	P	P		
Restart calculation						P	P	P	C	O	P	P

Summary

- Ample opportunity exists for collaboration with the NEAMS program. Forthcoming technical presentations and relate discussions should lead to identification of specifics topic areas.

- In addition to national laboratory collaborations, NEAMS invests >$5M in university-led R&D. May be possible to utilize some of that investment to support US-UK university collaboration.

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Clean. Reliable. **Nuclear.**

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NEAMS National Technical Director

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DOE-NE Program Overview and Timescales

NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

US DOE Mod Sim Overview and Outlook

Modest (and obvious proposal): initiate collaboration between UK-US by focusing on research efforts already supported (or likely to be supported).

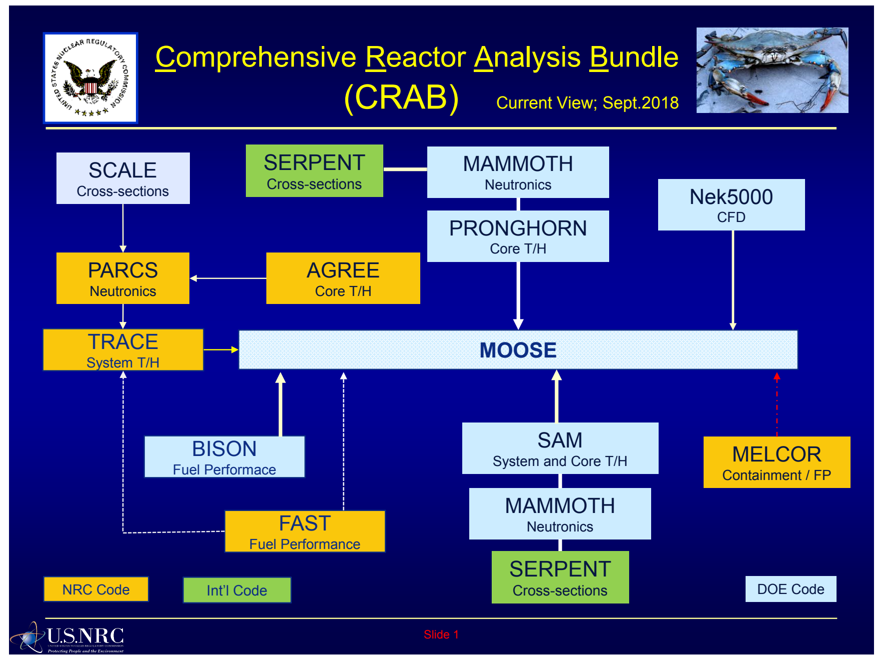
DOE-NE likely to continue support of advanced mod-sim through single centralized program combining capabilities of CASL (LWR) and NEAMS (non-LWR) programs.

Primary customers of US DOE mod sim efforts:

* NRC,
* LWR vendors and utilities,
* advanced reactor vendors,
* other DOE-NE programs.

R&D priorities (and timing of them) dictated by end user requirements, and are therefore highly dependent on reactor design, i.e. LWR focus more on operation, and non-LWR focus more on licensing.

Near term: ATF, "aging", CRAB, microreactors, FHRs



slide courtesy of Steve Bajorek (RES) – and slightly updated from NRC Non-Light Water Reactor (Non-LWR) Vision and Strategy – Strategy 2 Near- Term Implementation Action Plan Progress Report for Fiscal Year 2017 (ML17319A550)